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# Mixture effect on ionic selectivity and permeability of nanotubes

## Supplementary information

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Table S1 The number of ions in simulation systems.

| Nanopore | Solution conditions | Number of $K^+$ ions | Number of $Ca^{2+}$ ions | Number of $Cl^-$ ions |
|---|---|---|---|---|
| CNT | Single salt solution<br>1 M KCl | 44 | 0 | 30 |
| | Single salt solution<br>1 M $CaCl_2$ | 0 | 44 | 74 |
| | Mixed salt solution<br>(1 M KCl and 1 M $CaCl_2$) | 44 | 44 | 118 |
| PET | Single salt solution<br>1 M KCl | 92 | 0 | 78 |
| | Single salt solution<br>1 M $CaCl_2$ | 0 | 92 | 170 |
| | Mixed salt solution<br>(1 M KCl and 1 M $CaCl_2$) | 92 | 92 | 262 |

Table S2 Average permeability of $K^+$ ions and $Ca^{2+}$ ions of different concentrations in CNTs.

| | 0.5 M KCl | 1 M KCl | 2 M KCl | 3 M KCl(*) | 4 M KCl | 0.5 M $CaCl_2$ | 1 M $CaCl_2$ | 1.3 M $CaCl_2$ (*) |
|---|---|---|---|---|---|---|---|---|
| Permeability (ions/35 ns) | 115 | 196 | 547 | 790 | 1057 | 23 | 16 | 15 |

* The ionic strength of 4 M KCl solution or 1.3 M $CaCl_2$ solution is equal to that of the mixed salt solution of 1 M KCl and 1 M $CaCl_2$.

Table S3 Average loading time and passing time of $K^+$ ions and $Ca^{2+}$ ions in CNTs.

| Time (ns) | $K_s^+$ | $K_m^+$ | $Ca_s^{2+}$ | $Ca_m^{2+}$ |
|---|---|---|---|---|
| Loading | 0.13 | 0.12 (0.18*) | 1.17 | 0.20 (0.61*) |
| Passing | 0.11 | 0.10 | 0.50 | 0.09 |

* Time elapsed between two subsequently loading ions of the same type.

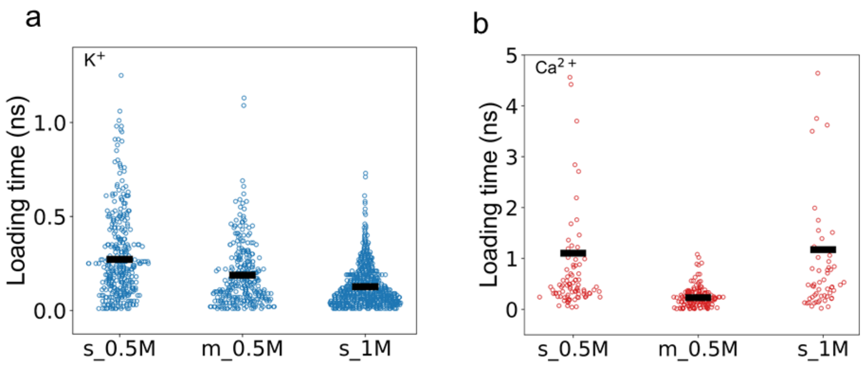

**Fig. S1** Concentration dependence on the loading time. (a-b) The loading time of $K^+$ (a) or $Ca^{2+}$ (b) ions into CNTs in the single salt solution with the concentration of 0.5 M (s_0.5M) and 1 M (s_1M) KCl (a) or $CaCl_2$ (b), and in mixed salt solution with 0.5 M KCl and 0.5 M $CaCl_2$ (m_0.5M). The range of *y*-axis is constrained to better view.

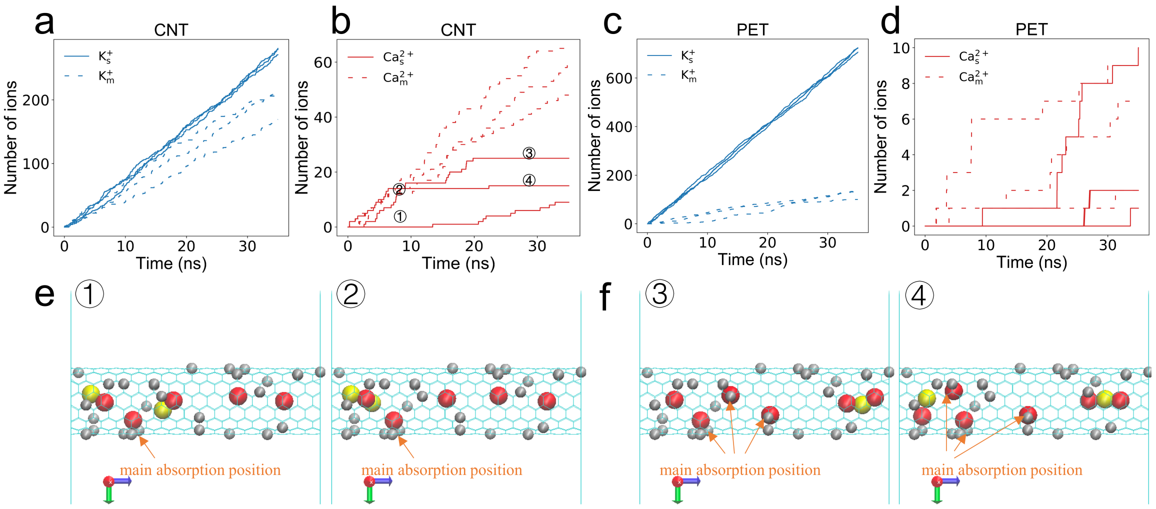

**Fig. S2** The number of transported ions through nanotubes as a function of the simulation time. (a, b) Ion flux of $K^+$ (a) and $Ca^{2+}$ (b) ions transporting through CNT. (c, d) Ion flux of $K^+$ (c) and $Ca^{2+}$ (d) ions transporting through PET nanopores. Solid lines and dash lines denote the single salt solution and mixed salt solution, respectively. (e, f) Representative snapshots of unblocked flow of $Ca^{2+}$ ions (e) corresponding to ① and ② in the linear rising line in (b), and blocked flow of $Ca^{2+}$ ions (f) corresponding to ③ and ④ in the plateaus in (b) in the CNT. The $Ca^{2+}$ ions are shown in red, the $Cl^-$ ions are shown in yellow, the charged C atoms are shown in gray.

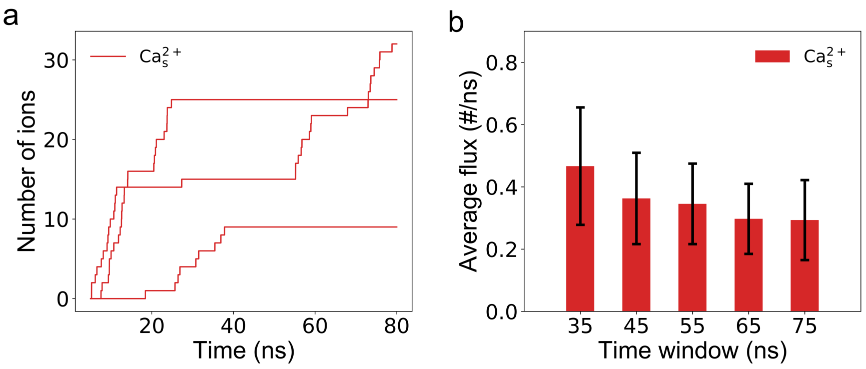

**Fig. S3** Accurate permeability rate of $Ca^{2+}$ ions in single salt solutions may need longer simulation time. (a) Ion flux of $Ca^{2+}$ ions in single slat solution (1 M $CaCl_2$) during an 80 ns simulation (b) The permeability rate of $Ca^{2+}$ ions slightly decreases in longer time windows.

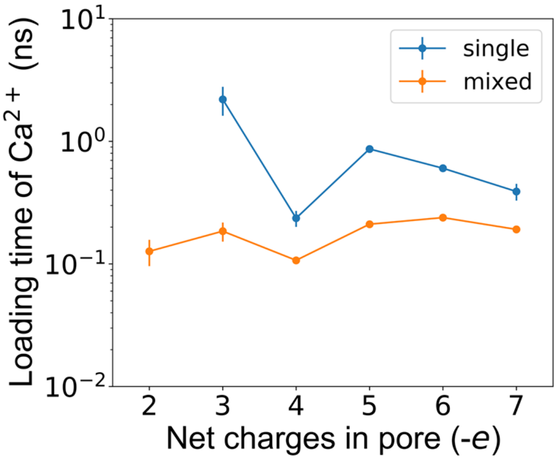

**Fig. S4** The loading time is uncorrelated with the total net charge number inside the CNT. Error bars represent standard errors.

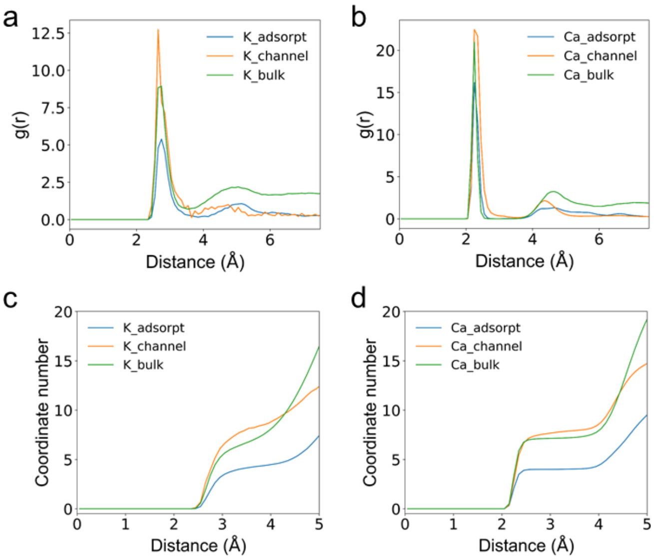

**Fig. S5** Comparison of the hydration status of the ions in the bulk (green), and inside CNTs moving (orange) or adsorbed (blue). (a-b) The radial distribution of hydration water molecules of $K^+$ ions (a) and $Ca^{2+}$ ions (b). (c-d) The accumulated hydration water molecules as a function of the distance from the $K^+$ ions (c) and $Ca^{2+}$ ions (d).

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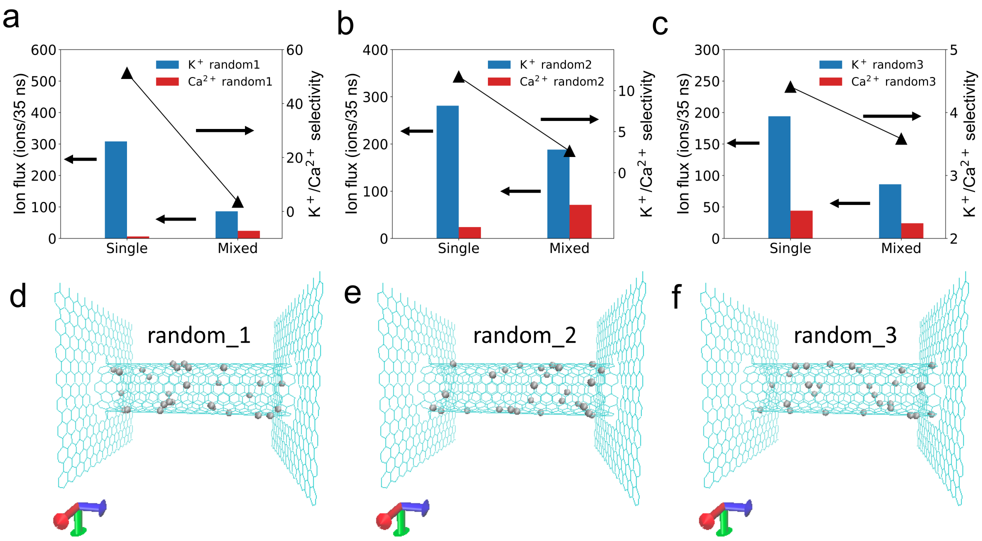

**Fig. S6** Ion flux and selectivity under different charge distributions. (a-c) Ion flux and selectivity of 3 other randomly charged CNTs. (d-f) The charge distribution of the above 3 CNTs. Charged carbon atoms are shown in gray balls.

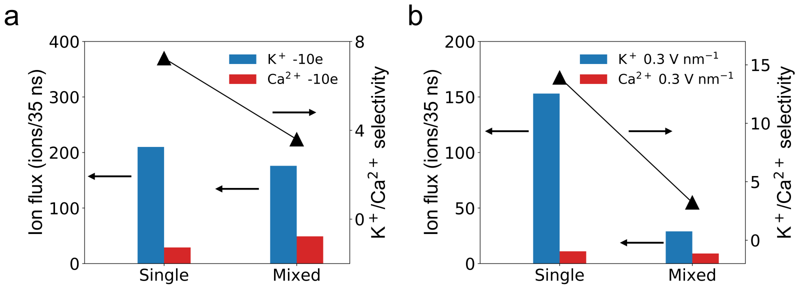

**Fig. S7** Ion flux and selectivity with a reduced surface charge density (a) and electric field (b).

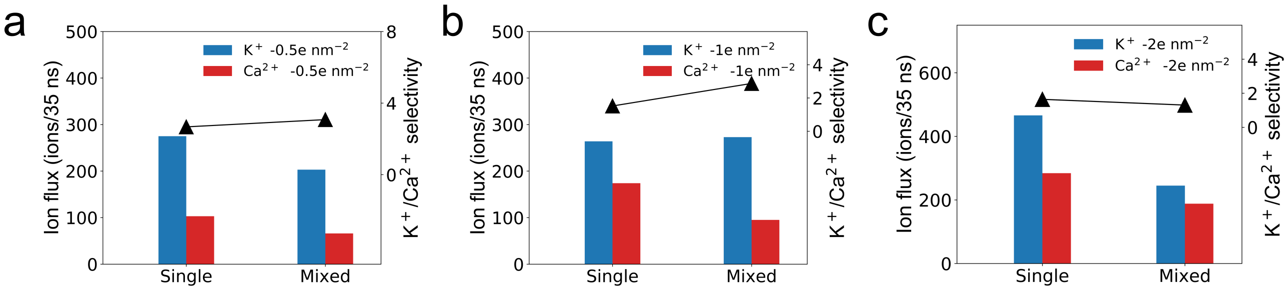

**Fig. S8** Ion flux and selectivity of uniformly charged CNTs with different surface charge densities of -0.5 e nm$^{-2}$ (a), -1 e nm$^{-2}$ (b), and -2 e nm$^{-2}$ (c).

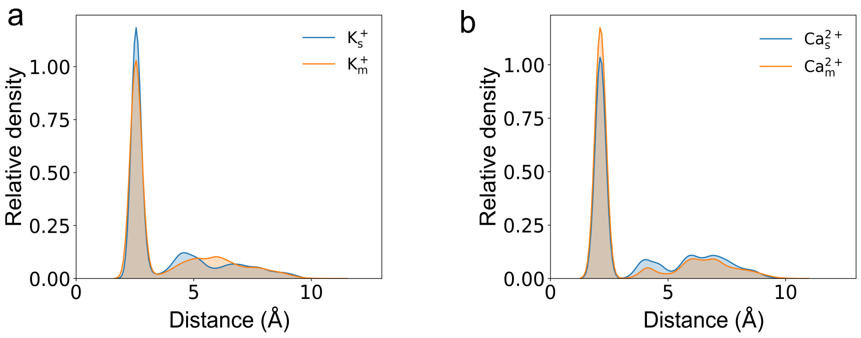

**Fig. S9** The radial distribution of ions inside the PET nanopore. (a, b) radial distribution of K$^+$ (a) and Ca$^{2+}$ (b) ions inside the PET nanopore in the single salt solution or mixed salt solution.

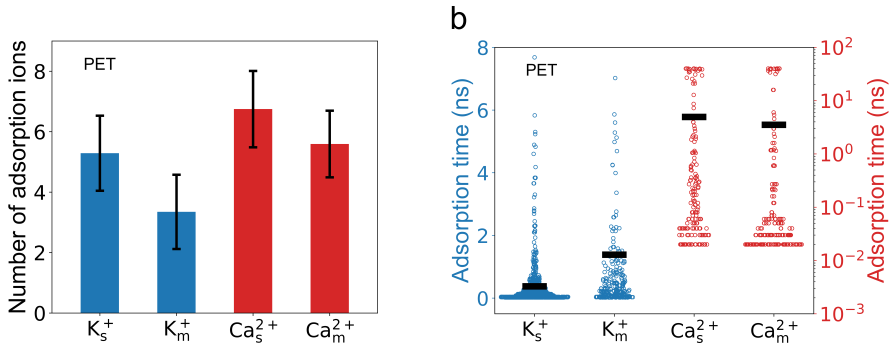

**Fig. S10** Ion adsorption in PET nanopores. (a) The number of adsorbed K$^+$ and Ca$^{2+}$ ions in PET nanopores. (b) Scatter plots of adsorption time of K$^+$ and Ca$^{2+}$ ions in PET nanopores.

**Movie S1** 22.5 ns simulation of $CaCl_2$ transporting through the charged CNT. The Ca$^{2+}$ and Cl$^-$ ions are shown in red and yellow, respectively. The charged C atoms are shown in gray. The snapshots shown in Fig. S1e ② and Fig. S1f ④ are extracted from this movie at 2.5 ns and 25 ns, respectively.